

# Construction of highly stable parallel two-step Runge–Kutta methods for delay differential equations

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## Abstract

It is shown that any  $A$ -stable two-step Runge–Kutta method of order  $\tilde{p}$  and stage order  $q = \tilde{p}$  for ordinary differential equations can be extended to the  $P$ -stable method of uniform order  $p = \tilde{p}$  for delay differential equations.

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## 1. Introduction

Consider the initial-value problem for a system of delay differential DDEs

$$\begin{cases} y'(t) = f(t, y(t), z(t)), & t \in [t_0, T], \\ y(t) = g(t), & t \in [\tau, t_0], \end{cases} \quad (1.1)$$

$\tau \leq t_0 < T$ , where  $f : R \times R^v \times R^v \rightarrow R^v$  is continuous and satisfies the Lipschitz condition with respect to the second and third argument. Here,  $g$  is a given initial function, and  $z(t)$  is defined by

$$z(t) = [y_1(\alpha_1(t)) \ y_2(\alpha_2(t)) \ \cdots \ y_v(\alpha_v(t))]^T,$$

with delay functions  $\alpha_i(t)$  such that  $\tau \leq \alpha_i(t) \leq t$ . Such systems form models for many real life applications in population dynamics, control theory, electrodynamics, viscoelasticity, biology, chemistry, and medical science and we refer to [12,16,24,25], or [30] for specific examples. The existence and uniqueness of solutions to (1.1) is discussed in [23].

Observe that each component  $y_i$  of  $y$  in (1.1) can depend only on one delay function  $\alpha_i(t)$ . This is not a very restrictive condition since systems of DDEs whose solution components depend on more than one delay can be brought into the form (1.1) by the process of “augmenting the system” described in [27] by introducing redundant components and enlarging the dimension of the original problem.

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To compute numerical approximation to the solution  $y$  of the problem (1.1) we consider the class of continuous two-step Runge–Kutta (TSRK) methods defined by

$$\begin{cases} Y_i^{[n]} = u_i y_h(t_{n-1}) + (1 - u_i) y_h(t_n) + h \sum_{j=1}^s (a_{ij} F_j^{[n-1]} + b_{ij} F_j^{[n]}), \\ y_h(t_n + \theta h) = \eta(\theta) y_h(t_{n-1}) + (1 - \eta(\theta)) y_h(t_n) + h \sum_{j=1}^s (v_j(\theta) F_j^{[n-1]} + w_j(\theta) F_j^{[n]}), \\ F_j^{[n-1]} = f(t_{n-1} + c_j h, Y_j^{[n-1]}, Z_j^{[n-1]}), \quad F_j^{[n]} = f(t_n + c_j h, Y_j^{[n]}, Z_j^{[n]}), \end{cases} \quad (1.2)$$

$i = 1, 2, \dots, s, n = 1, 2, \dots, N, \theta \in [0, 1], Nh = T - t_0$ , with given starting approximations  $y_h(t) \approx y(t)$  for  $t \in [\tau, t_1]$ ,  $Y_j^{[0]} \approx y(t_0 + c_j h)$ ,  $Z_j^{[0]} \approx z(t_0 + c_j h)$ ,  $j = 1, 2, \dots, s$  for some abscissa vector  $c = [c_1, \dots, c_s]^T$ . These starting approximations will be usually generated by a continuous RK method of sufficiently high order. In (1.2)  $s$  is the number of stages,  $t_n = t_0 + nh$ ,  $n = 0, 1, \dots, N$ ,  $y_h$  is an approximation to  $y$ ,  $Y_j^{[n]}$  are approximations to  $y(t_n + c_j h)$ ,  $Z_j^{[n]}$  are approximations to  $z(t_n + c_j h)$ ,  $j = 1, 2, \dots, s$ , and  $\eta(\theta)$ ,  $v_i(\theta)$ , and  $w_i(\theta)$  are polynomials such that  $\eta(0) = 0$ ,  $v_i(0) = 0$ , and  $w_i(0) = 0$ . The method (1.2) is zero-stable if and only if

$$-1 < \eta(1) \leq 1,$$

compare [20,21].

To lower the implementation costs of (1.2) and to make the method appropriate for parallel implementation we will assume that  $B$  is a diagonal matrix with a constant element  $\lambda$  on its diagonal. This method will be represented by the following table of its coefficients:

$$\begin{array}{c|c|c} u & A & B \\ \hline \eta(\theta) & v^T(\theta) & w^T(\theta) \end{array} = \begin{array}{c|ccc|ccc} u_1 & a_{11} & \cdots & a_{1s} & \lambda & & \\ \vdots & \vdots & \ddots & \vdots & & \ddots & \\ u_s & a_{s1} & \cdots & a_{ss} & & & \lambda \end{array}.$$

$$\begin{array}{c|ccc|ccc} \eta(\theta) & v_1(\theta) & \cdots & v_s(\theta) & w_1(\theta) & \cdots & w_s(\theta) \end{array}$$

However, most of our discussion is also valid for TSRK methods where the matrix  $B$  is arbitrary.

The discrete version of these methods corresponding to  $\theta = 1$  was introduced by Jackiewicz and Tracogna [20] in the context of ordinary differential equations (ODEs), and variable stepsize continuous TSRK methods for ODEs were investigated in [21]. The construction of TSRK methods with desirable stability properties was discussed in [20,2] where examples of highly stable ( $A$ -stable and  $L$ -stable) methods appropriate for stiff systems of ODEs were also presented. A different approach for the construction of TSRK methods appropriate for non-stiff problems was employed in [5,11] and their continuous extensions of order three were discussed in [6], where the results of numerical tests on a number of delay differential equations were also provided. An approach to the derivation of embedded pairs of TSRK formulas was described in [22]. Construction of stiffly accurate TSRK methods and their continuous extensions was discussed in a recent paper [7]. Stability properties of (1.2) for DDEs with respect to the test equation

$$\begin{cases} y'(t) = ay(t) + by(t - \tau), & t \geq 0, \\ y(t) = g(t), & t \in [-\tau, 0], \end{cases} \quad (1.3)$$

where  $a$  and  $b$  are complex parameters,  $\tau > 0$  is a constant delay and  $g$  a given initial function were discussed in [4]. The asymptotic stability of this equation was investigated by Barwell [8] and Zennaro [34].

The results about the convergence, order and stability of TSRK methods for ODEs and DDEs will be briefly reviewed and extended in Sections 2 and 3. In Section 4 we review the construction of  $A$ -stable TSRK methods for ODEs. In Sections 5–7 the methods (1.2) for DDEs with  $s$  stages are constructed which are highly stable with respect to the test equation (1.3) and convergent with uniform order  $p = s + 1$  and stage order  $q = p$ . In Section 8 some numerical experiments are presented which demonstrate high accuracy of new methods. Finally, in Section 9 some concluding remarks are given.

## 2. Convergence and order of TSRK methods for ODEs and DDEs

The TSRK method (1.2) applied to the system of ODEs  $y'(t) = f(t, y(t))$ ,  $t \in [t_0, T]$ , has a discrete order of convergence  $\tilde{p}$  if

$$\max\{\|y(t_n) - y_n\| : n = 0, 1, \dots, N\} = O(h^{\tilde{p}}),$$

where  $y_n := y_h(t_n)$ , uniform order of convergence  $p$  if

$$\sup\{\|y(t) - y_h(t)\| : t \in [t_0, T]\} = O(h^p)$$

and stage order of convergence  $q$  if

$$\max\{\|y(t_n + c_i h) - Y_i^{[n]}\| : n = 0, 1, \dots, N-1, i = 1, 2, \dots, s\} = O(h^q),$$

as  $h \rightarrow 0$ . It was demonstrated in [21,32,33] that the TSRK methods for ODEs with  $q = \tilde{p}$  have many desirable properties such as a possibility of continuous interpolants of order  $p = \tilde{p}$  and existence of asymptotically correct estimators of the local discretization error without any additional function evaluations in a step. Moreover, as observed in [15,33], such methods do not require starting procedure compatible with (1.2) and we can compute  $y_h(t) \approx y(t)$  for  $t \in [t_0, t_1]$  and  $Y_i^{[0]} \approx y(t_0 + c_i h)$ ,  $i = 1, 2, \dots, s$  by any continuous RK method of order  $\tilde{p}$ . This technique was employed in the algorithm based on explicit TSRK method of order  $\tilde{p} = 5$  and stage order  $q = 5$  for nonstiff systems of ODEs described in [3]. Additional advantage of methods with  $\tilde{p} = q$  is the avoidance of order reduction phenomenon [31,13,14] while integrating stiff systems of ODEs and DDEs which degrades the performance of methods with low stage order such as diagonally implicit or singly diagonally implicit RK methods [28,1,14].

Following [21] we define the error constants of (1.2) by

$$C_k = \frac{c^k}{k!} - \frac{(-1)^k u}{k!} - \frac{A(c-e)^{k-1}}{(k-1)!} - \frac{Bc^{k-1}}{(k-1)!} \quad (2.1)$$

and

$$\widehat{C}_k(\theta) = \frac{\theta^k}{k!} - \frac{(-1)^k \eta(\theta)}{k!} - \frac{v^T(\theta)(c-e)^{k-1}}{(k-1)!} - \frac{w^T(\theta)c^{k-1}}{(k-1)!}, \quad (2.2)$$

where  $e = [1 \dots 1]^T \in R^s$ , and  $c^k$  stands for componentwise multiplication. The result below generalizes [21, Theorem 3] and can be proved using standard techniques used in numerical solution of DDEs such as those presented, for example, in [9,17–19], or [35].

**Theorem 2.1.** Assume that  $y_h(t) = y(t) + O(h^p)$ ,  $t \in [\tau, t_1]$  and  $Y_i^{[0]} = y(t_0 + c_i h) + O(h^p)$ ,  $i = 1, 2, \dots, s$ , where the solution  $y$  to (1.1) is sufficiently smooth. Assume also that

$$\begin{cases} C_k = 0, & k = 1, 2, \dots, p-1, \\ \widehat{C}_k(\theta) = 0, & k = 1, 2, \dots, p-1, \quad \theta \in [0, 1], \\ \widehat{C}_p(1) = 0. \end{cases} \quad (2.3)$$

Then the method (1.2) is convergent with uniform order  $p$  and stage order  $q = p$ .

In the case of ODEs the discrete variant of Theorem 2.1 states that if

$$y_0 = y(t_0) + O(h^{\tilde{p}}), \quad y_1 = y(t_1) + O(h^{\tilde{p}}), \quad Y_i^{[0]} = y(t_0 + c_i h) + O(h^{\tilde{p}}),$$

$i = 1, 2, \dots, s$ , and if

$$\begin{cases} C_k = 0, & k = 1, 2, \dots, \tilde{p}-1, \\ \widehat{C}_k(1) = 0, & k = 1, 2, \dots, \tilde{p}, \end{cases} \quad (2.4)$$

then the TSRK method for ODEs is convergent with a discrete order  $\tilde{p}$  and stage order  $q = \tilde{p}$ .

### 3. Stability of TSRK methods for DDEs and uniform convergence of $P$ -stable methods

To investigate stability properties of TSRK methods for DDEs we apply (1.2) to the test equation (1.3) with a constant stepsize  $h = \tau/m$ , where  $m$  is a positive integer. This results in a sequence

$$\{y_n(m; \alpha, \beta)\}_{n=0}^{\infty},$$

$\alpha = ha$ ,  $\beta = hb$ , where  $y_n(m; \alpha, \beta) \approx y(t_n)$ . The region of stability  $\mathcal{S}$  of (1.2) is a subset of  $C \times C$  given by

$$\mathcal{S} = \{(\alpha, \beta) : y_n(m; \alpha, \beta) \rightarrow 0 \text{ as } n \rightarrow \infty \text{ for every } m\},$$

compare [4]. Here,  $C$  stands for the set of complex numbers. The method (1.2) is said to be  $P$ -stable if

$$\{(\alpha, \beta) : |\beta| < -\operatorname{Re}(\alpha)\} \subset \mathcal{S}.$$

As explained in [4] this means that if the method (2.1) is  $P$ -stable then the numerical solution  $y_n(m; \alpha, \beta) \rightarrow 0$  as  $n \rightarrow \infty$  for every  $m$  if  $y(t) \rightarrow 0$  as  $t \rightarrow \infty$ , where  $y(t)$  is the solution to (1.3).

Stability properties of TSRK methods (1.2) for DDEs with respect to (1.3) were investigated in [4]. Put

$$\begin{aligned}\tilde{u} &= [\eta_1, \eta_2, \dots, \eta_s]^T, & \eta_i &= \eta(c_i), \\ \Gamma &= [\gamma_{ij}]_{i,j=1}^s, & \gamma_{ij} &= v_j(c_i), \\ \Delta &= [\delta_{ij}]_{i,j=1}^s, & \delta_{ij} &= w_j(c_i).\end{aligned}$$

The main result of [4] is the following theorem which reduces  $P$ -stability of TSRK method for DDEs to  $A$ -stability of TSRK formulas for ODEs.

**Theorem 3.1.** Assume that the TSRK method for ODEs such that  $\tilde{u} = u$ ,  $\Gamma = A$ , and  $\Delta = B$  is  $A$ -stable. Then the corresponding TSRK method (1.2) for DDEs is  $P$ -stable.

This theorem suggests a way to construct  $P$ -stable TSRK methods for DDEs. We start with an  $A$ -stable method of order  $\tilde{p}$  and stage order  $q = \tilde{p}$  for ODEs

$$\begin{array}{c|c|c} u & A & B \\ \hline \eta & v^T & w^T \end{array} \quad (3.1)$$

and then compute continuous weights  $\eta(\theta)$ ,  $v_i(\theta)$ , and  $w_i(\theta)$ ,  $i = 1, 2, \dots, s$ , such that  $\eta(0) = 0$ ,  $\tilde{u} = u$ ,  $\eta(1) = \eta$ ,  $v_i(0) = 0$ ,  $\Gamma = A$ ,  $v_i(1) = v_i$ ,  $w_i(0) = 0$ ,  $\Delta = B$ , and  $w_i(1) = w_i$ . This leads to the linear system of equations for the coefficients of the polynomials  $\eta(\theta)$ ,  $v_i(\theta)$ , and  $w_i(\theta)$ . It follows then from Theorem 3.1 that the resulting TSRK method for DDEs

$$\begin{array}{c|c|c} u & A & B \\ \hline \eta(\theta) & v^T(\theta) & w^T(\theta) \end{array} \quad (3.2)$$

is  $P$ -stable. The order of uniform convergence of this method is given by the following theorem.

**Theorem 3.2.** Assume that the discrete  $s$ -stage TSRK method (3.1) for ODEs with  $c_i \neq 0$ ,  $c_i \neq 1$ ,  $c_i \neq c_j$  for  $i \neq j$ , has order  $\tilde{p}$  and stage order  $q = \tilde{p}$ . Assume also that the continuous weights  $\eta(\theta)$ ,  $v(\theta)$ , and  $w(\theta)$  of the method (3.2) are polynomials of degree less than or equal to  $s + 1$  such that

$$\begin{aligned}\eta(0) &= 0, & \eta(c_i) &= u_i, & \eta(1) &= \eta, \\ v_i(0) &= 0, & v_i(c_j) &= a_{ji}, & v_i(1) &= v_i, \\ w_i(0) &= 0, & w_i(c_j) &= b_{ji}, & w_i(1) &= w_i,\end{aligned}$$

$i, j = 1, 2, \dots, s$ . Then the continuous TSRK method (3.2) for DDEs is convergent with uniform order  $p = \tilde{p}$ .

**Proof.** It follows from the assumptions of the theorem that the error constants  $\tilde{C}_k(\theta)$  defined by (2.2) are polynomials of degree less than or equal to  $s + 1$ . We have also

$$\begin{aligned}\tilde{C}_k(0) &= 0, \\ \tilde{C}_k(c_j) &= \frac{c_j^k}{k!} - \frac{(-1)^k \eta(c_j)}{k!} - \frac{v(c_j)(c-e)^{k-1}}{(k-1)!} - \frac{w(c_j)c^{k-1}}{(k-1)!} \\ &= \frac{c_j^k}{k!} - \frac{(-1)^k u_j}{k!} - \frac{r_j(A)(c-e)^{k-1}}{(k-1)!} - \frac{r_j(B)c^{k-1}}{(k-1)!} \\ &= C_{k,j} = 0, \\ \tilde{C}_k(1) &= \frac{1}{k!} - \frac{(-1)^k \eta(1)}{k!} - \frac{v(1)(c-e)^{k-1}}{(k-1)!} - \frac{w(1)c^{k-1}}{(k-1)!} \\ &= \frac{1}{k!} - \frac{(-1)^k \eta}{k!} - \frac{v(c-e)^{k-1}}{(k-1)!} - \frac{wc^{k-1}}{(k-1)!} = 0,\end{aligned}$$

$k = 1, 2, \dots, \tilde{p}-1, j = 1, 2, \dots, s$ , where we have used the fact that the method (3.1) has stage order  $q = \tilde{p}$ . Here,  $r_j(A)$  stands for the  $j$ th row of  $A$  and  $C_{k,j}$  is the  $j$ th component of the error vector  $C_k$  defined by (2.1). Since  $\deg(\tilde{C}_k(\theta)) \leq s + 1$  it follows that  $\tilde{C}_k(\theta) \equiv 0, k = 1, 2, \dots, \tilde{p}-1$ , and as the consequence the method (3.2) is convergent with uniform order  $p = \tilde{p}$ .  $\square$

To ensure that the TSRK methods are also zero-stable we will always assume in this paper that  $\eta(\theta) \equiv 0$ . Then the condition  $\tilde{u} = u$  implies that  $u = 0$ .

#### 4. Construction of A-stable TSRK methods for ODEs

It was demonstrated in [2] that the TSRK method (3.1) for ODEs can be reformulated as a general linear method [10] of the form

$$\begin{bmatrix} Y \\ y^{[n+1]} \end{bmatrix} = \begin{bmatrix} A_1 & B_1 \\ A_2 & B_2 \end{bmatrix} \begin{bmatrix} hf(Y) \\ y^{[n]} \end{bmatrix}, \quad (4.1)$$

$n = 1, 2, \dots, N-1$ , where

$$Y = \begin{bmatrix} Y_1^{[n-1]} \\ \vdots \\ Y_s^{[n-1]} \\ Y_1^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix}, \quad f(Y) = \begin{bmatrix} f(Y_1^{[n-1]}) \\ \vdots \\ f(Y_s^{[n-1]}) \\ f(Y_1^{[n]}) \\ \vdots \\ f(Y_s^{[n]}) \end{bmatrix}, \quad y^{[n]} = \begin{bmatrix} Y_1^{[n-1]} \\ \vdots \\ Y_s^{[n-1]} \\ y_{n-1} \\ y_n \end{bmatrix}$$

and

$$\begin{aligned}A_1 &= \begin{bmatrix} 0 & 0 \\ A & B \end{bmatrix}, \quad B_1 = \begin{bmatrix} I & 0 & 0 \\ 0 & u & e - u \end{bmatrix}, \\ A_2 &= \begin{bmatrix} A & B \\ 0 & 0 \\ v^T & w^T \end{bmatrix}, \quad B_2 = \begin{bmatrix} 0 & u & e - u \\ 0 & 0 & 1 \\ 0 & \eta & 1 - \eta \end{bmatrix}.\end{aligned}$$

To study stability properties of TSRK methods we apply (4.1) to the standard test equation

$$y'(t) = \xi y(t), \quad t \geq 0, \quad (4.2)$$

$\xi \in C$ . This leads to the recurrence relation

$$y^{[n+1]} = M(z)y^{[n]},$$

$n = 1, 2, \dots$ , where  $z = h\xi$  and the matrix  $M(z)$  is defined by

$$M(z) = B_2 + zA_2(I - zA_1)^{-1}B_1.$$

The stability properties of (4.1) with respect to (4.2) are determined by the location of the roots of the stability polynomial defined by

$$\tilde{p}(\omega, z) = \det(\omega I - M(z)).$$

The coefficients of this polynomial in  $\omega$  are rational functions with respect to  $z$  and to avoid rational expressions it is more convenient to work instead with a polynomial

$$p(\omega, z) = (1 - \lambda z)^s \tilde{p}(\omega, z),$$

which takes the form

$$p(\omega, z) = (1 - \lambda z)^s \omega^{s+2} - p_1(z)\omega^{s+1} + \dots + (-1)^{s+2}p_0(z),$$

where  $p_i(z)$  are polynomials with respect to  $z$ .

The method (4.1) is said to be  $A$ -stable if all the roots of  $p(\omega, z)$  are inside of the unit circle for  $z \in C^-$  (i.e., if  $p(\omega, z)$  is a Schur polynomial [26] for  $z \in C^-$ ). Since  $z$  ranges over a two-dimensional set this condition is, in general, rather difficult to verify. However, assuming that  $\lambda > 0$  the roots  $\omega_i$  of  $p(\omega, z)$  are analytic functions of  $z \in C^-$  and it follows from the maximum principle that  $p(\omega, z)$  is a Schur polynomial for  $z \in C^-$  if and only if the moduli of the roots of  $p(\omega, iy)$  are less than or equal to one for  $y \in R$ , i.e., if  $p(\omega, z)$  is a von Neumann polynomial [29] (stability on the imaginary axis). This condition is more manageable and can be verified using the stability criterion listed at the end of this section (Theorem 4.1). Observe that if  $\lambda < 0$  then the roots of  $p(\omega, z)$  have poles at  $z = 1/\lambda$  and the resulting TSRK methods cannot be  $A$ -stable. Hence, if we are interested only in  $A$ -stable methods we can assume that  $\lambda > 0$  without loss of generality.

Consider the polynomial

$$\phi(\omega) = a_k \omega^k + a_{k-1} \omega^{k-1} + \dots + a_1 \omega + a_0,$$

where  $a_i \in C$  and define the polynomials

$$\widehat{\phi}(\omega) = \bar{a}_0 \omega^k + \bar{a}_1 \omega^{k-1} + \dots + \bar{a}_{k-1} \omega + \bar{a}_k,$$

$$\phi_1(\omega) = \frac{1}{\omega} (\widehat{\phi}(0)\phi(\omega) - \phi(0)\widehat{\phi}(\omega)),$$

where  $\bar{a}_i$  is the complex conjugate of  $a_i$ . We have the following theorem (see [29]).

**Theorem 4.1.** *The function  $\phi(\omega)$  is a von Neumann polynomial if and only if either*

$$|\widehat{\phi}(0)| > |\phi(0)| \quad \text{and} \quad \phi_1(\omega) \quad \text{is a von Neumann polynomial}$$

or

$$\phi_1(\omega) \equiv 0 \quad \text{and} \quad \phi'(\omega) \quad \text{is a von Neumann polynomial.}$$

Applying this criterion successively to the polynomial  $p(\omega, z)$  leads to the algebraic conditions for  $A$ -stability of TSRK methods. Then starting with the  $A$ -stable methods for ODEs we can construct the  $P$ -stable methods for DDEs which are also uniformly convergent with order  $p = \tilde{p}$  using the approach presented in Section 3.

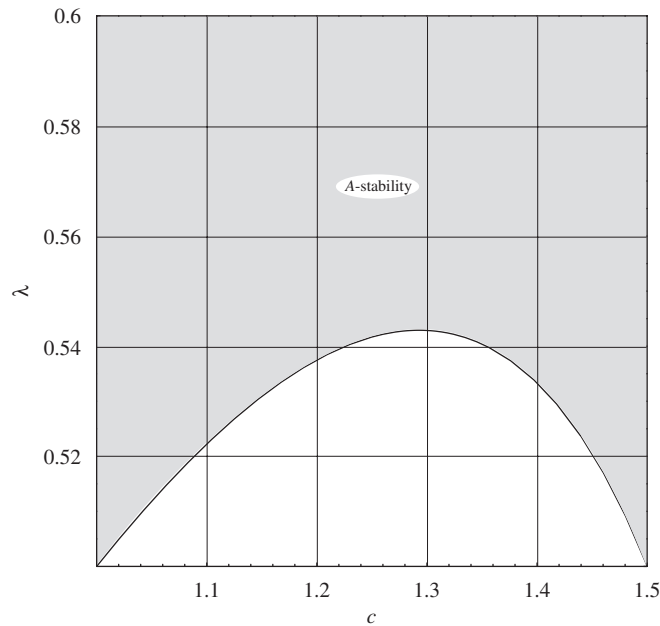


Fig. 1. Region of A-stability in the  $(c, \lambda)$ -plane for TSRK methods with  $s = 1$  and  $\tilde{p} = q = 2$ .

## 5. Construction of $P$ -stable TSRK methods for DDEs with $s = 1$ and $p = q = 2$

Assuming that  $\eta = 0$  and  $u = 0$  and solving the system (2.4) of order and stage order conditions for  $\tilde{p} = 2$  with respect to  $a, v$  and  $w$  we obtain a two parameter family of TSRK methods of order  $\tilde{p} = 2$  and stage order  $q = 2$  given by

$$\frac{u}{\eta} \left| \begin{array}{c|c|c} a & \lambda \\ \hline v & w \end{array} \right| = \frac{0}{0} \left| \begin{array}{c|c|c} c - \lambda & \lambda \\ \hline \frac{1}{2(2-c)} & \frac{3-2c}{2(2-c)} \end{array} \right|, \quad (5.1)$$

$c \neq 2$ . It can be verified using the stability criterion given in Theorem 4.1 in Section 4 that if the method (5.1) is A-stable then necessarily  $1 \leq c \leq \frac{3}{2}$  or  $c > 2$ . For  $1 \leq c \leq \frac{3}{2}$  this method is A-stable if and only if

$$\lambda \geq \frac{1 + 3c - 2c^2}{4(2 - c)}.$$

This region of A-stability is plotted in the  $(c, \lambda)$ -plane in Fig. 1.

To construct a continuous TSRK method for DDEs we assume that the continuous weights  $v(\theta)$  and  $w(\theta)$  have the form

$$v(\theta) = \theta(v_{11} + v_{12}\theta), \quad w(\theta) = \theta(w_{11} + w_{12}\theta),$$

$\theta \in [0, 1]$ . Solving the systems of linear equations

$$v(c) = a, \quad v(1) = v \quad (5.2)$$

and

$$w(c) = \lambda, \quad w(1) = w, \quad (5.3)$$

where  $a, \lambda, v$ , and  $w$  are defined in (5.1) leads to the continuous TSRK method

$$\frac{0}{0} \left| \begin{array}{c|c|c} c - \lambda & \lambda \\ \hline v(\theta) & w(\theta) \end{array} \right| \quad (5.4)$$

with  $v(\theta)$  and  $w(\theta)$  defined by

$$v(\theta) = \theta \left( \frac{4c - 3c^2 - (4 - 2c)\lambda}{2c(c-1)(c-2)} + \frac{2c^2 - 3c + (4 - 2c)\lambda}{2c(c-1)(c-2)} \theta \right),$$

$$w(\theta) = \theta \left( \frac{2c^3 - 3c^2 + (4 - 2c)\lambda}{2c(c-1)(c-2)} + \frac{3c - 2c^2 - (4 - 2c)\lambda}{2c(c-1)(c-2)} \theta \right),$$

$c \neq 1, c \neq 2$  (observe that  $c \neq 0$  since  $\lambda > 0 = v(0)$ ). It follows from Theorem 3.2 that the method (5.4) is convergent with uniform order  $p = 2$ .

For  $c = 1$  the systems (5.2) and (5.3) have a solution only if  $\lambda = \frac{1}{2}$  and the resulting methods are

$$\begin{array}{c|c|c} 0 & \frac{1}{2} & \frac{1}{2} \\ \hline 0 & (1-\gamma)\theta + (\gamma - \frac{1}{2})\theta^2 & \gamma\theta + (\frac{1}{2} - \gamma)\theta^2 \end{array}, \quad (5.5)$$

where  $\gamma$  is a free parameter. For  $\gamma = \frac{1}{2}$  the functions  $v(\theta)$  and  $w(\theta)$  are linear. Observe that for  $\theta = 1$  the method (5.5) takes the form

$$\begin{array}{c|c|c} 0 & \frac{1}{2} & \frac{1}{2} \\ \hline 0 & \frac{1}{2} & \frac{1}{2} \end{array},$$

and is equivalent to the trapezoidal rule for ODEs.

## 6. Construction of $P$ -stable TSRK methods for DDEs with $s = 2$ and $p = q = 3$

To construct TSRK methods with  $s = 2$  we will choose in advance the abscissa vector  $c = [c_1, c_2]^T$  where  $c_i \in [0, 1]$ ,  $i = 1, 2$ . We will illustrate below the construction of formulas with  $c_1 = \frac{1}{4}$  and  $c_2 = \frac{3}{4}$ . Assuming that  $\eta = 0$  and  $u = 0$  and solving the system (2.4) with  $\tilde{p} = 3$  we obtain a two parameter family of methods of order  $\tilde{p} = 3$  and stage order  $q = 3$ :

$$\begin{array}{c|c|c} u & A & B \\ \hline \eta & v^T & w^T \end{array} = \begin{array}{c|c|c} 0 & \frac{16\lambda-3}{16} & \frac{7-32\lambda}{16} \\ 0 & \frac{32\lambda-15}{16} & \frac{27-48\lambda}{16} \\ 0 & \frac{13-24w_2}{24} & \frac{36w_2-19}{12} \end{array} \begin{array}{c} \lambda \\ \lambda \\ w_2 \end{array}. \quad (6.1)$$

Using the stability criterion given in Theorem 4.1 we have performed a computer search looking for methods which are  $A$ -stable. The results of this search are displayed in Fig. 2 for  $-0.6 \leq w_2 \leq 0.4$  and  $0.6 \leq \lambda \leq 1.6$ .

To construct continuous TSRK methods for DDEs which are  $P$ -stable we look for continuous weights  $v_i(\theta)$  and  $w_i(\theta)$  in the form

$$v_i(\theta) = \theta(v_{i,1} + v_{i,2}\theta + v_{i,3}\theta^2),$$

$$w_i(\theta) = \theta(w_{i,1} + w_{i,2}\theta + w_{i,3}\theta^2),$$

$i = 1, 2, \theta \in [0, 1]$ . Solving the system of linear equations

$$v_i(c_j) = a_{ji}, \quad v_i(1) = v_i \quad (6.2)$$

and

$$w_i(c_j) = b_{ji}, \quad w_i(1) = w_i \quad (6.3)$$



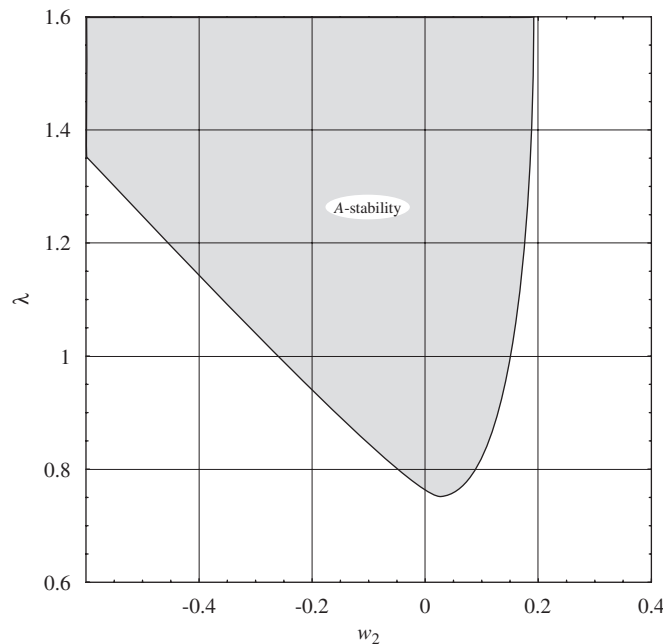


Fig. 2. Region of A-stability in the  $(w_2, \lambda)$ -plane for TSRK methods with  $s = 2$  and  $\tilde{p} = q = 3$ .

and  $i = 1, 2$ , leads to

$$\begin{aligned} v_1(\theta) &= \theta \left( \frac{37 + 64\lambda - 24w_2}{24} - \frac{107 - 72\lambda - 48w_2}{9}\theta + \frac{2(49 - 48\lambda - 24w_2)}{9}\theta^2 \right), \\ v_2(\theta) &= \theta \left( \frac{36w_2 - 31 - 96\lambda}{12} + \frac{205 - 24\lambda - 144w_2}{9}\theta - \frac{4(49 - 24\lambda - 36w_2)}{9}\theta^2 \right), \\ w_1(\theta) &= \theta \left( \frac{49 + 192\lambda - 72w_2}{24} - \frac{2(49 + 84\lambda - 72w_2)}{9}\theta + \frac{2(49 + 48\lambda - 72w_2)}{9}\theta^2 \right), \\ w_2(\theta) &= \theta \left( \frac{3w_2 - 8\lambda}{3} + \frac{8(5\lambda - 2w_2)}{3}\theta - \frac{16(2\lambda - w_2)}{3}\theta^2 \right). \end{aligned}$$

It follows from Theorem 3.1 that the methods with  $v_i(\theta)$  and  $w_i(\theta)$  given above are  $P$ -stable and it follows from Theorem 3.2 that they are convergent with uniform order  $p = 3$ .

Treating  $c_1$  and  $c_2$  as free parameters and allowing  $b_{2,1}$  to be nonzero (i.e., considering more general form of the coefficient matrix  $B$  than that in (6.1)) we can also construct 2-stage TSRK methods of order  $\tilde{p} = 4$  and stage order  $q = 4$  by solving the corresponding system of order and stage order conditions given by (2.4). The coefficients of the resulting formulas are complicated functions of  $c_1$  and  $c_2$  and are not reproduced here. In Fig. 3 we present the results of computer search for A-stable methods for  $0.4 \leq c_1 \leq 1.4$  and  $2 \leq c_2 \leq 3$ . Choosing, for example,  $c_1 = \frac{3}{4}$  and  $c_2 = \frac{9}{4}$  the method takes the form

$$\begin{array}{c|c|c} u & A & B \\ \hline \eta & v^T & w^T \end{array} = \begin{array}{c|cc|cc} 0 & \frac{3}{16} & -\frac{3}{16} & \frac{3}{4} & & \\ 0 & -\frac{3}{16} & -\frac{15}{16} & \frac{21}{8} & \frac{3}{4} & \\ 0 & \frac{107}{720} & -\frac{43}{144} & \frac{161}{144} & \frac{23}{720} & \end{array}.$$

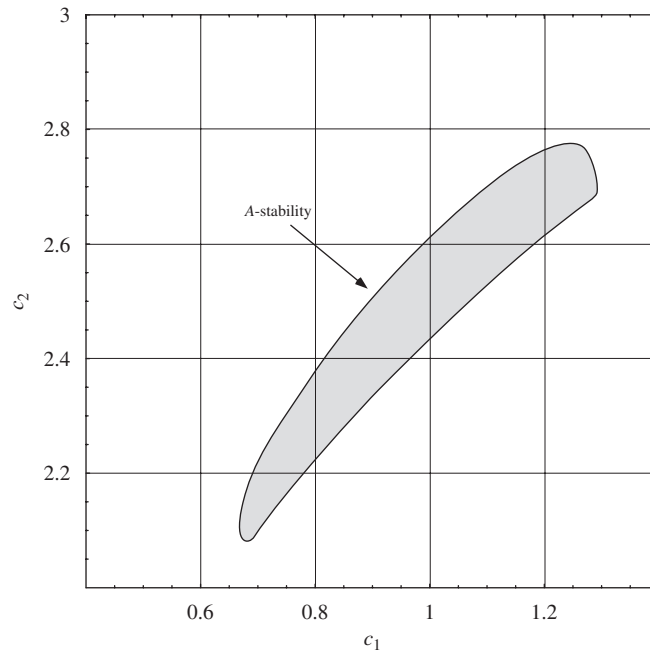


Fig. 3. Region of A-stability in the  $(c_1, c_2)$ -plane for TSRK methods with  $s = 2$  and  $\tilde{p} = q = 4$ .

The continuous weights  $v_i(\theta)$  and  $w_i(\theta)$  of the TSRK method for DDEs which is  $P$ -stable and convergent with uniform order  $p = 4$  are

$$v_1(\theta) = \theta \left( \frac{797}{1200} - \frac{149}{225}\theta + \frac{11}{75}\theta^2 \right), \quad v_2(\theta) = \theta \left( -\frac{13}{240} - \frac{14}{45}\theta + \frac{1}{15}\theta^2 \right),$$

$$w_1(\theta) = \theta \left( \frac{103}{240} + \frac{44}{45}\theta - \frac{13}{45}\theta^2 \right), \quad w_2(\theta) = \theta \left( -\frac{47}{1200} - \frac{1}{225}\theta + \frac{17}{225}\theta^2 \right).$$

These weights were computed from (6.2) and (6.3). The disadvantage of this method is that  $c_2 \notin [0, 1]$  and that  $B$  is not diagonal.

### 7. Construction of $P$ -stable TSRK methods for DDEs with $s = 3$ and $p = q = 4$

Choosing  $c = [\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]^T$ ,  $\eta = 0$ ,  $u = 0$ , and solving (2.3) with  $\tilde{p} = 4$  with respect to  $a_{ij}$ , and  $v_1, v_2, w_1, w_2$  leads to a family of methods of order  $\tilde{p} = 4$  and stage order  $q = 4$  which depend on free parameters  $v_3, w_3$ , and  $\lambda$ . We compute next  $v_3$  so that the stability function of the resulting method has the form

$$p(\omega, z) = \omega^2((1 - \lambda z)^3 \omega^3 - p_2(z)\omega^2 + p_1(z)\omega - p_0(z)),$$

i.e.,  $\omega = 0$  is a double root of  $p(\omega, z)$ . Here,  $p_0(z)$ ,  $p_1(z)$  and  $p_2(z)$  are polynomials of degree less than or equal to three. This leads to TSRK methods of the form

0	$\frac{23-14\lambda}{48}$	$\frac{4(6\lambda-1)}{3}$	$\frac{53-288\lambda}{48}$	$\lambda$			
0	$\frac{19-72\lambda}{12}$	$\frac{5(18\lambda-5)}{6}$	$\frac{37-120\lambda}{12}$	$\lambda$			
0	$\frac{57-160\lambda}{16}$	$3(8\lambda - 3)$	$\frac{3(33-80\lambda)}{16}$	$\lambda$			
0	$v_1$	$v_2$	$v_3$		$w_1$	$w_2$	$w_3$

(7.1)

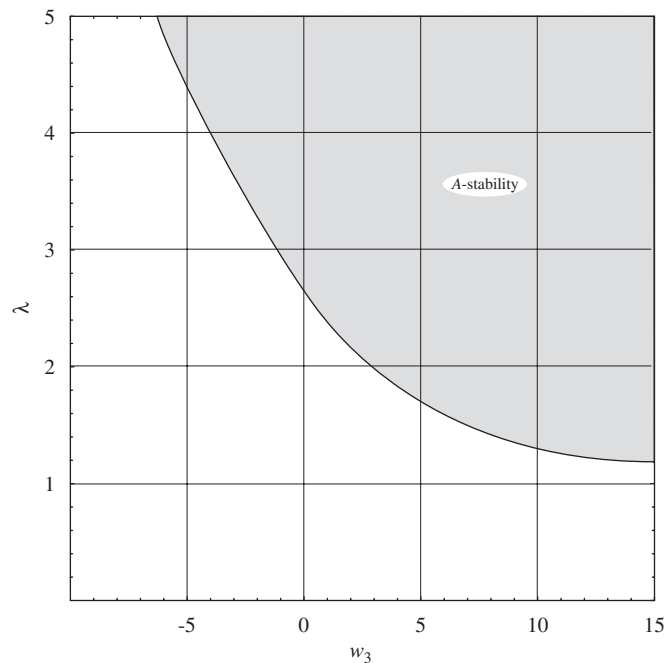


Fig. 4. Region of A-stability in the  $(w_3, \lambda)$ -plane for TSRK methods with  $s = 3$  and  $\tilde{p} = q = 4$ .

where

$$\begin{aligned}
 v_1 &= -\frac{39 - 158\lambda + 96\lambda^2 + 576\lambda^3 - 72w_3 + 336\lambda w_3 - 576\lambda^2 w_2}{24(4\lambda - 1)(6\lambda - 1)}, \\
 v_2 &= \frac{179 - 630\lambda + 96\lambda^2 + 2880\lambda^3 - 336w_2 + 1440\lambda w_3 - 2304\lambda^2 w_3}{36(4\lambda - 1)(6\lambda - 1)}, \\
 v_3 &= -\frac{5(31 - 78\lambda - 96\lambda^2 + 576\lambda^3 - 60w_3 + 216\lambda w_3 - 288\lambda^2 w_3)}{36(4\lambda - 1)(6\lambda - 1)}, \\
 w_1 &= \frac{83 + 330\lambda - 2208\lambda^2 + 2880\lambda^3 - 120w_3 - 720\lambda w_3 + 2880\lambda^2 w_3}{72(4\lambda - 1)(6\lambda - 1)}, \\
 w_2 &= -\frac{29 - 522\lambda + 1536\lambda^2 - 576\lambda^3 - 48w_3 + 864\lambda w_3 - 2304\lambda^2 w_3}{36(4\lambda - 1)(6\lambda - 1)}.
 \end{aligned}$$

In Fig. 4 we display the region in the  $(w_3, \lambda)$ -plane for  $-10 \leq w_3 \leq 15$  and  $0 \leq \lambda \leq 5$ , which corresponds to TSRK methods which are A-stable.

Using the approach described in Section 3 we can also construct TSRK methods for DDEs which are continuous extensions of (7.1). The example of such method corresponding to  $w_3 = \frac{9}{2}$  and  $\lambda = 2$  is listed below:

$$\begin{array}{c|ccc|ccc}
 0 & -\frac{265}{48} & \frac{44}{3} & -\frac{523}{48} & 2 & & \\
 0 & -\frac{125}{12} & \frac{155}{6} & -\frac{203}{12} & & 2 & \\
 0 & -\frac{263}{16} & 39 & -\frac{381}{16} & & & 2 \\
 \hline
 0 & v_1(\theta) & v_2(\theta) & v_3(\theta) & w_1(\theta) & w_2(\theta) & w_3(\theta)
 \end{array} \quad (7.2)$$

Here,  $v_i(\theta)$  and  $w_i(\theta)$  given by

$$\begin{aligned}v_1(\theta) &= \theta \left( -\frac{97201}{1848} + \frac{54557}{252}\theta - \frac{103850}{231}\theta^2 + \frac{199076}{693}\theta^3 \right), \\v_2(\theta) &= \theta \left( \frac{375433}{2772} - \frac{200293}{378}\theta + \frac{732964}{693}\theta^2 - \frac{1384616}{2079}\theta^3 \right), \\v_3(\theta) &= \theta \left( -\frac{269635}{2772} + \frac{132673}{378}\theta - \frac{444676}{693}\theta^2 + \frac{804344}{2079}\theta^3 \right), \\w_1(\theta) &= \theta \left( \frac{117637}{5544} - \frac{45061}{756}\theta + \frac{13514}{693}\theta^2 + \frac{61676}{2079}\theta^3 \right), \\w_2(\theta) &= \theta \left( -\frac{33137}{2772} + \frac{24065}{378}\theta - \frac{43844}{693}\theta^2 - \frac{1016}{2079}\theta^3 \right), \\w_3(\theta) &= \theta \left( \frac{37}{6} - \frac{125}{3}\theta + \frac{232}{3}\theta^2 - \frac{112}{3}\theta^3 \right).\end{aligned}$$

It follows again from Theorem 3.1 that the method (7.2) is  $P$ -stable and it follows from Theorem 3.2 that this method is convergent with uniform order  $p = 4$ .

## 8. Numerical experiments

To demonstrate the behavior of the obtained methods we have implemented an experimental code for the 3-stage method (7.2) of order 4 and its continuous extension given in Section 7. We applied this code to the following two examples of delay differential equations:

**Example 1** (*Oregonator* [12]).

$$\begin{cases} y_1'(t) = 0.0804y_2(t) - 1.6 \cdot 10^9 y_1(t)y_2(t - 0.15) + 480y_1(t) - 8 \cdot 10^7 (y_1(t))^2, \\ y_2'(t) = -0.0804y_2(t) - 1.6 \cdot 10^9 y_1(t)y_2(t - 0.15) + 480y_1(t), \end{cases} \quad (8.1)$$

$t \in [0, 100.5]$ . The initial conditions are  $y_1(t) = 10^{-10}$  and  $y_2(t) = 10^{-5}$  for  $t \leq 0$ .

**Example 2** (*4D enzyme kinetics with an inhibitor molecule* [30]).

$$\begin{cases} y_1'(t) = 10.5 - \frac{y_1(t)}{1 + 0.0005y_4(t-4)^3}, \\ y_2'(t) = \frac{y_1(t)}{1 + 0.0005y_4(t-4)^3} - y_2(t), \\ y_3'(t) = y_2(t) - y_3(t), \\ y_4'(t) = y_3(t) - \frac{1}{2}y_4(t), \end{cases} \quad (8.2)$$

$t \in [0, 160]$ . The initial conditions are  $y(t) = [60, 10, 10, 20]^T$  for  $t \leq 0$ .

The absolute and relative errors at the endpoints of corresponding intervals of integration for the stepsize  $h = 0.0011$  (for both examples) are given in Table 1. The graphs of the solutions are presented in Fig. 5 for Example 1 and in Fig. 6 for Example 2. These results confirm high accuracy of the TSRK formulas constructed in this paper.

## 9. Concluding remarks

We described an approach to the construction of highly stable ( $P$ -stable) TSRK methods for DDEs of uniform order of convergence  $p = \tilde{p}$  and stage order  $q = \tilde{p}$ , where  $\tilde{p}$  is the order of the underlying formula for ODEs. In this approach we start with any  $A$ -stable TSRK method for ODEs which is usually found by a computer search using the stability

Table 1  
Examples 1, 2—absolute and relative errors at the end points

$h = 0.0011$	$y_1$	$y_2$	$y_3$	$y_4$
Example 1				
abs. error	9.2112e−14	2.6090e−11	—	—
rel. error	3.3497e−04	7.3307e−05	—	—
Example 2				
abs. error	7.5895e−03	2.6563e−04	2.3262e−03	4.6185e−03
rel. error	2.2371e−04	1.1698e−05	1.2353e−04	2.0743e−04

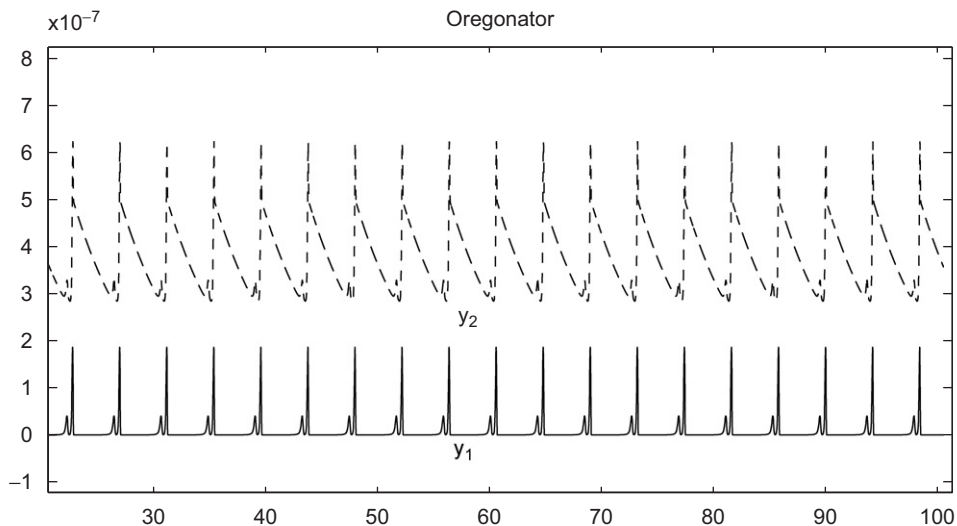


Fig. 5. The graph of the solution of Oregonator problem obtained by TSRK method with  $s = 3$  and  $\tilde{p} = q = 4$  for  $h = 0.0011$ .

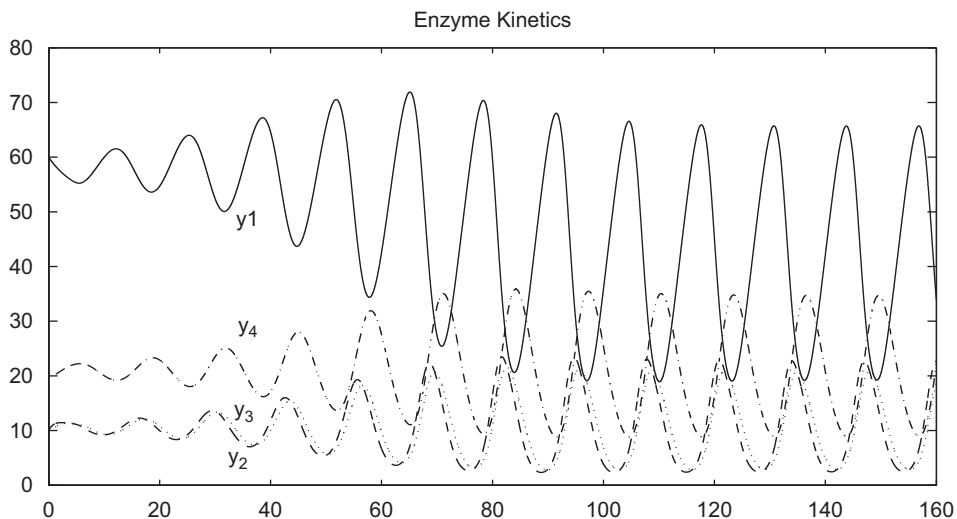


Fig. 6. The graph of the solution of enzyme kinetics problem obtained by TSRK method with  $s = 3$  and  $\tilde{p} = q = 4$  for  $h = 0.0011$ .

criterion which determines the location of the roots of the corresponding stability function (Theorem 4.1 in Section 4). Then we compute the continuous weights  $v(\theta)$  and  $w(\theta)$  of the TSRK method for DDEs by solving the linear systems of equations for their coefficients. As explained in Section 3 the resulting methods are then  $P$ -stable and convergent

with the uniform order  $p$  equal to the order  $\tilde{p}$  of the corresponding formula for ODEs. This approach is illustrated for TSRK methods for DDEs with  $s + 1 = \tilde{p} = p = q$  for  $s = 1, 2$ , and 3, where  $s$  is the number of stages. The numerical results illustrate high accuracy of formulas obtained in this paper.

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